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C:\Program Files\Stnexp\Queries\154r.str
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chain nodes :
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ring nodes :
   1 2 3 4 5 6 7 8 9 11 12 13 14 15 16 17 18 19 20 21 22
ring/chain nodes :
   23
chain bonds :
   8-13 9-20
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 11-12 11-16 12-13 13-14 14-15
   15-16 17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
   5-7: 6-9 7-8 8-9 9-20
exact bonds :
   8-13
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 17-18 17-22
   18-19 19-20 20-21 21-22
isolated ring systems :
   containing 1 : 11 : 17 :
G1: [*1], [*2], [*3], [*4]
Match level :
   1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:Atom 12:Atom
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13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:Atom 21:Atom

22:CLASS 23:CLASS 24:CLASS 25:CLASS 30:CLASS 31:CLASS 32:CLASS

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         FEB 28
                 data from INPADOC
        FEB 28
                BABS - Current-awareness alerts (SDIs) available
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                MEDLINE/LMEDLINE reloaded
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     7
        MAR 02
                GBFULL: New full-text patent database on STN
        MAR 03
NEWS 8
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NEWS
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                MEDLINE file segment of TOXCENTER reloaded
                KOREAPAT now updated monthly; patent information enhanced
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     10 MAR 22
                Original IDE display format returns to REGISTRY/ZREGISTRY
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NEWS 13 MAR 22
                REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS 14 APR 04
                EPFULL enhanced with additional patent information and new
                 fields
NEWS 15 APR 04
                EMBASE - Database reloaded and enhanced
                New CAS Information Use Policies available online
NEWS 16 APR 18
NEWS 17 APR 25
                Patent searching, including current-awareness alerts (SDIs),
                based on application date in CA/CAplus and USPATFULL/USPAT2
                may be affected by a change in filing date for U.S.
                applications.
NEWS 18 APR 28
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                U.S. patent records in CA/CAplus
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                GBFULL enhanced with patent drawing images
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                REGISTRY has been enhanced with source information from
                 CHEMCATS
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     21 MAY 26
                STN User Update to be held June 6 and June 7 at the SLA 2005
                Annual Conference
NEWS EXPRESS
             JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
             MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP)
             AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
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=>
Uploading C:\Program Files\Stnexp\Queries\154r.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 07:27:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 350 TO ITERATE

100.0% PROCESSED 350 ITERATIONS 12 ANSWERS

8122

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5878 TO

PROJECTED ANSWERS: 32 TO 446

L2 12 SEA SSS SAM L1

=> s l1 full

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100.0% PROCESSED 6399 ITERATIONS

284 ANSWERS

SEARCH TIME: 00.00.01

L3 284 SEA SSS FUL L1

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=> s 12/thu

12 L2

683031 THU/RL

L4 4

4 L2/THU

(L2 (L) THU/RL)

=> s 14 and inflammation?

133132 INFLAMMATION?

L5 0 L4 AND INFLAMMATION?

=> d l4, ibib abs hitstr, 1-4

L4 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:526062 HCAPLUS

DOCUMENT NUMBER: 135:107328

TITLE: Preparation of 1,2-diarylbenzimidazolealkanoates and

analogs for treatment of disorders mediated by

microglia activation

INVENTOR(S): Kuhnke, Joachim; Halfbrodt, Wolfgang; Moenning, Ursula

PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 141 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

					KIND DATE			APPLICATION NO.						DATE				
WO								WO 2001-EP334					20010112					
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BE	BG	, BR,	BY,	ΒZ,	CA,	CH,	CN,	
		CR,	CU,	CZ,	DK,	DM,	DZ,	EE,	ES,	FI	, GB	GD,	GE,	GH,	GM,	HR,	HU,	
		ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR	, KZ	, LC,	LK,	LR,	LS,	LT,	LU,	
		LV,	ΜA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ	, NO	NZ,	PL,	PT,	RO,	RU,	SD,	
		SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT	TZ, TZ	, UA,	UG,	UZ,	VN,	ΥU,	ZA,	
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	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ	, TZ	, UG,	ZW,	AT,	BE,	CH,	CY,	
•		DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙΊ	LU, LU	, MC,	NL,	PT,	SE,	TR,	BF,	
		ΒJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML	, MR	, NE,	SN,	TD,	TG			
						CA 2001-2396227												
BR	BR 2001007628																	
EP	1246	1246808			A1 20021009			EP 2001-915133										
	R:						ES,					, LI,	LU,	NL,	SE,	MC,	PT,	
							RO,											
JP	JP 2003523961																	
EE	EE 200200390							EE 2002-390										
NZ	5193	26							NZ 2001-519326									
US	US 2002006948,				A1 20020117				US 2001-759360						20010116			
	1068						2003									0020	613	
NO	NO 2002003362															0020	712	
	ZA 2002006470				Α		2004	0219								0020		
PRIORIT	PRIORITY APPLN. INFO.:									DE	2000	-1000	2898		A 2	0000	114	
	• ~										2000					0000		
	ρq									WO	2001	-EP33	4		W 2	0010	112	
OTHER S	OTHER SOURCE(S):					PAT	135:	10732	28									

$$\begin{array}{c|c}
R^3 & & \\
N & & R^2 \\
R & & R^1 & I
\end{array}$$

GI

AB Title compds. [I; R = ZZ1R4; R1,R2 = (un)substituted (hetero)aryl; R3 = H, halo, substituted alkyl, alkoxy, etc.; R4 = CO2H, alkoxycarbonyl, CONH2, SO3H, etc.; Z = O, (alkyl)imino, acylimino; Z1 = (heteroatom-interrupted) alkyl(en)ylene, etc.] were prepared Thus, I (R1 = R2 = Ph, R3 = H)(II; R = 6-OH) was etherified by BrCH2CO2CHMe3 to give II (R = 6-OCH2CO2CHMe3). Data for biol. activity of I were given.

IT 350232-45-0P 350233-02-2P RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 1,2-diarylbenzimidazolealkanoates and analogs for treatment of disorders mediated by microglia activation)

350232-45-0 HCAPLUS RN

Hexanoic acid, 6-[[5-[[(4-bromophenyl)sulfonyl]amino]-1,2-diphenyl-1H-CN benzimidazol-6-yl]oxy]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 350233-02-2 HCAPLUS

Benzenesulfonamide, 4-bromo-N-[(4-bromophenyl)sulfonyl]-N-(1,2-diphenyl-1H-CN benzimidazol-5-yl) - (9CI) (CA INDEX NAME)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

T.4 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:623154 HCAPLUS

DOCUMENT NUMBER: 127:293221

TITLE: Methods of treating or preventing interstitial

cystitis using substituted benzimidazoles

INVENTOR(S): Iyengar, Smriti; Muhlhauser, Mark A.; Thor, Karl B.

PATENT ASSIGNEE(S): Eli Lilly and Company, USA; Iyengar, Smriti;

Muhlhauser, Mark A.; Thor, Karl B.

SOURCE: PCT Int. Appl., 121 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

> PATENT NO. KIND DATE APPLICATION NO. DATE WO 9733873 19970918 WO 1997-US3895 A1 AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, TJ, TM, TR,

TT, UA, UG, US, UZ, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, KE, LS, MW, SD, SZ, UG, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG 19970918 CA 1997-2248013 19970307 CA 2248013 AA AU 9722078 **A1** 19971001 AU 1997-22078 19970307 T2 JP 2000506529 20000530 JP 1997-532805 19970307 US 1998-125956 US 6025379 20000215 19980825 PRIORITY APPLN. INFO.: US 1996-13129P 19960311 WO 1997-US3895 19970307 OTHER SOURCE(S):

MARPAT 127:293221

Ι

GT

$$R^3$$
 R^2 R^1

The invention provides methods for the treatment or prevention of AB interstitial cystitis or urethral syndrome using substituted benzimidazoles I [R1, R2 = H, alkyl, alkoxy, (un) substituted Ph, cycloalkyl, naphthyl, heterocyclyl, phenylalkyl, heterocyclylalkoxy, etc.; R3 = H, NO2, CF3, halo, alkanoyl, amino, alkyl, alkoxy, alkylthio, cycloalkyl, (un) substituted heterocyclyl, amino, aminoalkoxy, aminoalkyl, heterocyclylalkyl, heterocyclylalkoxy, etc.; only 1 or R1 and R2 may be H] or their pharmaceutically acceptable salts or solvates. Approx. 170 synthetic examples of I are given, with the products serving as target compds. and/or intermediates. Use of specific preferred compds. containing cyclic or acyclic amine sidechains is also claimed. For instance, etherification of 1-benzyl-2-(3,4,5-trimethoxyphenyl)-6hydroxybenzimidazole-HCl (preparation given) with 4-(2-chloroethyl)morpholine-HCl in acetone in the presence of K2CO3 gave preferred title compound II. Methods for the bioassay and clin. evaluation of I are described (no data).

ΙI

IT 175714-04-2P, 1-Phenyl-2-(4-chlorophenyl)-5-[1-(ethylamino)ethyl]benzimidazole maleate RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (product and/or intermediate; preparation of benzimidazole derivs. for treatment of interstitial cystitis)

175714-04-2 HCAPLUS RN

·1H-Benzimidazole-5-methanamine, 2-(4-chlorophenyl)-N-ethyl- α -methyl-1-phenyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM

CRN 175714-03-1

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

L4

GI

ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:563632 HCAPLUS

DOCUMENT NUMBER: 125:300996

TITLE: Preparation of benzimidazoles useful for treating

physiological disorders associated with β -amyloid

peptide

INVENTOR(S): Lunn, William H. W.; Monn, James A.; Zimmerman, Dennis

Μ.

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: U.S., 30 pp.

CODEN: USXXAM DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5552426 ∜	Α	19960903	US 1994-235400	19940429
PRIORITY APPLN. INFO.:	•		US 1994-235400	19940429
OTHER SOURCE(S):	MARPAT	125:300996	·	•

$$R^3$$
 N N R^2 N

AB The title compds. [I; R1 = H, alkoxy, (un) substituted alkyl, (un) substituted Ph, (un) substituted naphthyl, (un) substituted cycloalkyl; R2 = H, alkyl, alkoxy, (un) substituted Ph, (un) substituted naphthyl, etc.; R3 = H, alkanoyl, amino, alkyl, cycloalkyl, halogen, alkylthio, CF3, etc.] [e.g., 1-phenyl-2-[3,4-dimethylphenyl]-6-[2-(1-

piperidinyl)ethoxy]benzimidazole], which are useful in treating or preventing conditions associated with β -amyloid peptide (e.g., Alzheimer's disease, Down's syndrome, etc.), are prepared and I-containing formulations presented.

IT 175714-04-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzimidazoles useful for treating physiol. disorders associated with β -amyloid peptide)

RN 175714-04-2 HCAPLUS

CN 1H-Benzimidazole-5-methanamine, $2-(4-\text{chlorophenyl})-N-\text{ethyl}-\alpha-\text{methyl}$ 1-phenyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

175714-03-1 CRN CMF C23 H22 C1 N3.

CM.

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1996:252224 HCAPLUS

DOCUMENT NUMBER:

124:289536

TITLE:

Preparation of benzimidazole derivatives as non-peptide tachykinin receptor antagonists

INVENTOR(S):

Burns, Robert Frederick, Jr.; Gitter, Bruce Donald;

Monn, James Allen; Zimmerman, Dennis Michael

PATENT ASSIGNEE(S):

Eli Lilly and Co., USA

SOURCE:

Can. Pat. Appl., 143 pp.

CODEN: CPXXEB

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2148053	AA	19951030	CA 1995-2148053	19950427
CA 2148053 EP 694535	A1	19960131	EP 1995-302707	19950424

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ZA	9503	311			Α	1	1996	1024	:	ZA	1995-	-3311			1	99504	124
BR	9501	770			Α	1	1995	1121	1	BR	1995	-1770			1	99504	125
AU	9517	656			A1	1	1995	1109	1	UA	1995	-1765	6		1	99504	126
CN	1113	236			Α	1	1995	1213	(CN	1995	-1047	25		1	99504	126
NO	9501	613			Α	1	1995	1030	1	ОИ	1995-	-1613			1	99504	127
FI	9502	064			Α	1	1995	1030	1	FI	1995	-2064			1	99504	128
HU	7063	7			A2	1	1995	1030	1	HU	1995	-1249			1	99504	128
JP	0810	9169			A2]	1996	0430		JP	1995-	-1052	97		1	99504	128
PRIORITY	APP	LN.	INFO	.:					1	US	1994	-2354	01	1	A 1	99404	129
OTHER SO	URCE	(S):			CAS	REACT	r 12	4:289	9536	; M	ARPA:	Г 124	:289	536			
GI																	

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I; R1, R2 = H, C1-C12 alkyl, C1-C6 alkoxy, etc.; R3 = H, NO2, C1-C6 alkanoyl, etc.], useful in treatment of CNS disorders, acute and chronic obstructive airway diseases, inflammatory diseases, allergies, cutaneous diseases, etc., were prepared and formulated. Condensation of 4,3-H2N(O2N)C6H3OH with 3,4,5-(MeO)3C6H2COCl in PhNMe2/PhMe followed by reaction of the intermediate II with PhCHO under H2 in the presence of Pd/C in DMF, cyclization of the intermediate III using POCl3/CHCl3, deprotection of the 6-OH group with 1N NaOH/THF and acidification with 1N HCl afforded I.HCl [R1 = 3,4,5-(MeO)3C6H2; R2 = PhCH2; R3 = 6-OH] which showed IC50 of 1.130 μ M against binding to human NK-1 receptor in cultured cell assays.

IT 175714-04-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of benzimidazole derivs. as non-peptide tachykinin receptor antagonists)

RN 175714-04-2 HCAPLUS

CN 1H-Benzimidazole-5-methanamine, 2-(4-chlorophenyl)-N-ethyl- α -methyl-1-phenyl-, (2Z)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

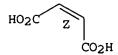
CM 1

CRN 175714-03-1 CMF C23 H22 C1 N3

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.



=> file caold

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L1 STRUCTURE UPLOADED

L2 12 S L1

L3 284 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 07:28:03 ON 27 MAY 2005

L4 4 S L2/THU

L5 0 S L4 AND INFLAMMATION?

FILE 'CAOLD' ENTERED AT 07:28:29 ON 27 MAY 2005

=> s 13

L6 1 L3

=> d 16, all, 1

L6 ANSWER 1 OF 1 CAOLD COPYRIGHT 2005 ACS on STN

AN CA55:16523h CAOLD

TI chemotherapeutic amidines - (XVIII) substituted 4,4'-diamidinodiphenylamines

AU Easson, A. P. T.

```
ΙT
    5469-66-9 24293-28-5 42772-85-0 95202-37-2 100537-93-7 100540-44-1
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    112552-11-1 112949-86-7 113038-13-4 114186-80-0 114329-37-2 114840-05-0
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SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION

0.00

-2.92

FILE 'REGISTRY' ENTERED AT 07:29:04 ON 27 MAY 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 MAY 2005 HIGHEST RN 851163-60-5 DICTIONARY FILE UPDATES: 25 MAY 2005 HIGHEST RN 851163-60-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

```
E3
             1 --> 102703-74-2/RN
E4
                   102703-75-3/RN
             1
E5
                   102703-76-4/RN
             1
E6
                   102703-77-5/RN
             1
E7
                   102703-78-6/RN
             1
E8
                   102703-79-7/RN
             1
E9
                   102703-80-0/RN
             1
E10
             1
                   102703-81-1/RN
E11
             1
                   102703-82-2/RN
E12
                   102703-83-3/RN
=> s e3
L7
             1 102703-74-2/RN
=> d 17
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
L7
RN
     102703-74-2 REGISTRY
ED
     Entered STN: 14 Jun 1986
     5-Benzimidazolecarbonitrile, 1-(p-cyanophenyl)-2-phenyl- (6CI) (CA INDEX
CN
     NAME)
FS
     3D CONCORD
     C21 H12 N4
MF
     CAOLD
SR
     STN Files:
                  BEILSTEIN*, CA, CAOLD, CAPLUS
LC
         (*File contains numerically searchable property data)
```

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)